Free energy variational approach for the classical anisotropic XY model in a crystal field

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A variational approach for the free energy is used to study the three-dimensional anisotropic XY model in the presence of a crystal field. The magnetization and the phase diagrams as a function of the parameters of the Hamiltonian are obtained. Some limiting results for isotropic XY and planar rotator models in two and three dimensions are analyzed and compared to previous results obtained from analytical approximations as well as from those obtained from more reliable approaches such as series expansion and Monte Carlo simulations. It is also shown that from this general variational approach some simple assumptions can drastically simplify the self-consistent implicit equations. The validity of the low temperature region of this approach is analyzed and compared to Monte Carlo results as well.

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1. INTRODUCTION

Ising and Heisenberg models are spin Hamiltonians which have been originally proposed in the study of magnetism in pure and diluted materials [1, 2, 3, 4]. They are widely studied and employed in both classical and quantum contexts. However, a great interest has also been devoted to the XY model due to the richness of its phase diagram and the character of its transition [5, 6]. In particular, the XY model in two dimensions is of prime interest in the field of statistical mechanics because of its intriguing and unusual phase transition. Recently, the study of the XY model has been motivated not only due to its applicability in describing real magnetic materials (for instance, it has been quite recently shown that the phase diagram of the compound $RbFe(MoO_4)_2$ is in good agreement with the theoretical predictions for a two-dimensional XY classical model [7]) but as well as in condensed matter systems, for example liquid crystals [8] and superconductors [9, 10, 11], among others.

The one-dimensional version of the quantum spin-1/2 XY model has been exactly solved by Lieb, Shultz and Mattis [12]. Although the quantum nature of real magnets cannot be forgotten, the study of classical models continues to be an important subject of research. The two-dimensional classical version of the XY model has been treated by Berezinskii and Kosterlitz and Thouless [5, 6] and they showed that the vortices and anti-vortices play a central role in the thermodynamic behavior of the model. For higher dimensions this model (as well as a planar rotator version) has been studied through approximate analytical techniques [13, 14, 15, 16] and Monte Carlo simulations [17]. In addition, classical models in general, and in particular the XY model, have become very popular recently in the context of quantum phase transitions, where a d-dimensional quantum model at $T = 0$ is transformed into a classical $d + 1$ dimensional one [18, 19].

The effort for a better theoretical understanding of the high temperature superconductors has also lead to an increase in treating anisotropic XY type models [11, 20, 21, 22], specially its two-dimensional version. However, despite the layered structure of these systems, the high temperature superconductors are not strictly two dimensional. For this reason, inter layer interaction should be important in describing their thermodynamic properties [11], as well as the inclusion of possible crystal field interactions.

In this work we study the classical anisotropic XY model with a crystal field interaction described by the following Hamiltonian

$$\begin{aligned}\mathcal{H} &= -J \sum_{\langle \vec{r},\vec{r}' \rangle} \{S^x_{\vec{r}} S^x_{\vec{r}'} + S^y_{\vec{r}} S^y_{\vec{r}'}\} \\ &- J_z \sum_{\langle \vec{r},\vec{r}' \rangle} \{S^x_{\vec{r}} S^x_{\vec{r}'} + S^y_{\vec{r}} S^y_{\vec{r}'}\} + D \sum_{\vec{r}} (S^z_{\vec{r}})^2 \ , \quad (1)\end{aligned}$$

where J is the exchange interaction between spins in the layers parallel to the xy plane and J_z the exchange interaction between spins in different adjacent layers. D is the crystal field and $S^\alpha_{\vec{r}}$ are the $\alpha = x, y, z$ components of a classical spin $|\vec{S}_{\vec{r}}| = 1$. The first sum runs on nearest neighbor spins $\langle \vec{r}, \vec{r}' \rangle$ within the layers and the second sum on nearest neighbor spins $\langle \vec{r}, \vec{r}' \rangle$ between layers (in order to avoid confusion here and in the following expressions, the subscript of the exchange interaction or the variational parameter in front of the sums will define whether the spins belong to the same layer or to adjacent layers). The last sum is made over the entire N spins on the simple cubic lattice.

The Hamiltonian (1) can be written in a more convenient form by means of a polar representation for the

spins [13, 14]

$$\vec{S_{\vec{r}}} = (S^x_{\vec{r}}, S^y_{\vec{r}}, S^z_{\vec{r}}) = (\sin\theta_{\vec{r}}\cos\phi_{\vec{r}}, \sin\theta_{\vec{r}}\sin\phi_{\vec{r}}, S^z_{\vec{r}}),$$
$$\vec{S_{\vec{r}}} = (\sqrt{1-(S^z_{\vec{r}})^2}\cos\phi_{\vec{r}}, \sqrt{1-(S^z_{\vec{r}})^2}\sin\phi_{\vec{r}}, S^z_{\vec{r}}) \ , \quad (2)$$

where $\theta_{\vec{r}}$ and $\phi_{\vec{r}}$ are the spherical angles of the spin at the site $\vec{r}$. In this representation the Hamiltonian given by Eq. (1) takes the form

$$\mathcal{H} = -\frac{J}{2}\sum_{\vec{r},\vec{a}}\sqrt{1-(S^z_{\vec{r}})^2}\sqrt{1-(S^z_{\vec{r}+\vec{a}})^2}\cos(\phi_{\vec{r}+\vec{a}}-\phi_{\vec{r}})$$
$$- \frac{J_z}{2}\sum_{\vec{r},\vec{c}}\sqrt{1-(S^z_{\vec{r}})^2}\sqrt{1-(S^z_{\vec{r}+\vec{c}})^2}\cos(\phi_{\vec{r}+\vec{c}}-\phi_{\vec{r}})$$
$$+ D\sum_{\vec{r}}(S^z_{\vec{r}})^2, \quad (3)$$

where $\vec{a}$ labels the four nearest-neighbor sites of $\vec{r}$ in the xy plane and $\vec{c}$ the two nearest-neighbor sites of $\vec{r}$ along the z direction.

The above model has been treated according to the self-consistent harmonic approximation (SCHA) in the case $D = 0$ for the three-dimensional model [16] as well as the planar rotator model [15] (in this case there is no z spin components). The approach in [16], however, only considers the cases $J_z \approx J$ and $J_z << J$, that is, quasi-isotropic case or weak layer coupling and no general treatment has been done for any value of $0 \leq J_z \leq J$.

In what concerns the theoretical approach, it is well known that the SCHA has been extensively used in the literature [11, 15, 16, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31]. It consists of replacing the original Hamiltonian (3) by a harmonic one by expanding the corresponding cosines to the second order with effective exchange constants that take into account the nonlinearities of the interactions. The effective couplings are then chosen to minimize the corresponding free energy of the system. In the present work we use a variational method based on Bogoliubov inequality for the free energy to study the model Hamiltonian (1) in order to obtain its low temperature thermodynamic properties. This procedure is the same as the SCHA employed in previous works. Some simplifications are also suggested in order to easier handle the awkward self-consistent implicit equations.

The plan of the paper is as follows. In the next section, we present the analytical procedure according to the variational approach for the free energy in order to obtain the thermodynamic properties of the model. In section 3, the numerical results are presented, where the role played by the anisotropy in the presence of a crystal field is shown to be for itself relevant (for instance, in the context of high temperature superconductors). Additional assumptions are also suggested which can make the implicit self-consistent equations easier to be handled. Some concluding remarks are discussed in section 4.

2. VARIATIONAL APPROACH FOR THE FREE ENERGY

The present variational approach is based on the Bogoliubov inequality for the free energy

$$F \leq F_0 + \langle \mathcal{H} - \mathcal{H}_0(\gamma)\rangle_0 \equiv \Phi(\gamma), \quad (4)$$

where $\mathcal{H}$ is the Hamiltonian in study given by Eq. (1) or (3), $\mathcal{H}_0(\gamma)$ is a trial Hamiltonian which can be exactly solved and depends on variational parameters γ. F is the free energy of the system described by $\mathcal{H}$, F_o is the free energy of the trial Hamiltonian $\mathcal{H}_o$, and the thermal average $< ... >_0$ is taken over the ensemble defined by $\mathcal{H}_0$. The approximate free energy is given by the minimum of $\Phi(\gamma)$ with relation to γ, that is, $F \equiv \Phi_{min}(\gamma)$.

In general, the trial Hamiltonian should resemble, in some aspects, the one under study. In this case, $\mathcal{H}_0$ can be chosen as a sum of two parts

$$\mathcal{H}_o = \mathcal{H}^{\phi}_o + \mathcal{H}^z_o, \quad (5)$$

in such a way that the first part is a kind of a planar Hamiltonian

$$\mathcal{H}^{\phi}_o = \frac{\gamma}{4}\sum_{\vec{r},\vec{a}}(\phi_{\vec{r}+\vec{a}}-\phi_{\vec{r}})^2 + \frac{\gamma_z}{4}\sum_{\vec{r},\vec{c}}(\phi_{\vec{r}+\vec{c}}-\phi_{\vec{r}})^2 \quad (6)$$

and the second term is an axial Hamiltonian

$$\mathcal{H}^z_o = (D + 2J + J_z)\sum_{\vec{r}}(S^z_{\vec{r}})^2, \quad (7)$$

where γ and γ_z stand for the variational parameters. This harmonic choice for $\mathcal{H}_0$ is also motivated by the fact that at low temperatures the angle differences $|\phi_{\vec{r}+\vec{a}} - \phi_{\vec{r}}| << 1$ and $|\phi_{\vec{r}+\vec{c}} - \phi_{\vec{r}}| << 1$ so the cosines in Eq. (3) can be expanded up to second order to give the terms $(\phi_{\vec{r}+\vec{a}} - \phi_{\vec{r}})^2$ and $(\phi_{\vec{r}+\vec{c}} - \phi_{\vec{r}})^2$ in $\mathcal{H}^{\phi}_0$. Since in this case there is a negligible variation in the z components of the spins, we can further assume that $S^z_{\vec{r}} \approx S^z_{\vec{r}+\vec{a}}$ and $S^z_{\vec{r}} \approx S^z_{\vec{r}+\vec{c}}$, so the square roots in Eq. (3) are eliminated and we end up to a term $D+2J+J_z$ in the corresponding axial term. Thus, it turns out that this approach will be valid only in the low temperature region.

Obtaining the averages regarding the trial Hamiltonian requires diagonalizing (5). The planar Hamiltonian $\mathcal{H}^{\phi}_0$ can be diagonalized in the reciprocal space through the Fourier transform of $\phi_{\vec{r}}$

$$\phi_{\vec{r}} = \frac{1}{\sqrt{N}}\sum_{\vec{q}} e^{-i\vec{q}\cdot\vec{r}}\phi_{\vec{q}}, \quad (8)$$

with the inverse transform $\phi_{\vec{q}}$ given by

$$\phi_{\vec{q}} = \frac{1}{\sqrt{N}}\sum_{\vec{r}} e^{i\vec{q}\cdot\vec{r}}\phi_{\vec{r}}. \quad (9)$$

Using the transformations (8) in Eq. (6) and the fact that the system is translationally invariant we get

$$\mathcal{H}_o^{\phi} = \frac{1}{2}\sum_{\vec{q}}\{\gamma\sum_{\vec{a}}(1-e^{-i\vec{q}\vec{a}})\phi_{\vec{q}}\phi_{-\vec{q}} + \gamma_z\sum_{\vec{c}}(1-e^{-i\vec{q}\vec{c}})\phi_{\vec{q}}\phi_{-\vec{q}}\}. \quad (10)$$

Summing now over the vectors $\vec{a}$ in the xy plane and $\vec{c}$ along the z direction and rearranging terms we obtain the diagonal form of the planar trial Hamiltonian

$$\mathcal{H}_o^{\phi} = \sum_{\vec{q}}(\gamma_q+\gamma_{qz})|\phi_q|^2, \quad (11)$$

where $\gamma_q = \gamma(2-\cos q_x a-\cos q_y a)$, $\gamma_{qz} = \gamma_z(1-\cos q_z c)$, $a=|\vec{a}|$, $c=|\vec{c}|$ and $|\phi_q|^2 = \phi_{\vec{q}}\phi_{-\vec{q}}$.

The diagonalizing of the axial term of the harmonic Hamiltonian (7) is obtained by introducing the corresponding Fourier transform of the z component of the spins $S_{\vec{r}}^z$

$$S_{\vec{r}}^z = \frac{1}{\sqrt{N}}\sum_{\vec{q}} e^{-i\vec{q}\cdot\vec{r}}S_{\vec{q}}^z, \quad (12)$$

and the inverse transform $S_{\vec{q}}^z$ given by

$$S_{\vec{q}}^z = \frac{1}{\sqrt{N}}\sum_{\vec{q}} e^{i\vec{q}\cdot\vec{r}}S_{\vec{r}}^z. \quad (13)$$

Applying (12) to Eq. (7) one gets

$$\mathcal{H}_o^z = (D+2J+J_z)\sum_{\vec{q}}|S_{\vec{q}}^z|^2, \quad (14)$$

where $|S_{\vec{q}}^z|^2 = S_{\vec{q}}^z S_{-\vec{q}}^z$.

The partition function $\mathcal{Z}_0$ can be computed by first noting that the planar and the axial parts of the harmonic Hamiltonian are independent so

$$\mathcal{Z}_0 = Tre^{-\beta\mathcal{H}_0} = Tre^{-\beta(\mathcal{H}_o^{\phi}+\mathcal{H}_o^z)} = \mathcal{Z}_0^{\phi}\mathcal{Z}_0^z. \quad (15)$$

Since both $\mathcal{H}_0^{\phi}$ and $\mathcal{H}_0^z$ are quadratic in their variables one has

$$\mathcal{Z}_o^{\phi} = Tre^{-\beta\mathcal{H}_o^{\phi}} = \prod_{\vec{q}}\left[\frac{\pi}{\beta(\gamma_q+\gamma_{qz})}\right]^{\frac{1}{2}} \quad (16)$$

and

$$\mathcal{Z}_o^z = Tre^{-\beta\mathcal{H}_o^z} = \prod_{\vec{q}}\left[\frac{\pi}{\beta\Omega}\right]^{\frac{1}{2}}, \quad (17)$$

where $\Omega = D+2J+J_z$. The free energy F_0 is then given by

$$F_0 = -\frac{k_BT}{2}\sum_{\vec{q}}\ln\frac{\pi}{\beta(\gamma_q+\gamma_{qz})} - \frac{k_BT}{2}N\ln\frac{\pi}{\beta\Omega} \quad (18)$$

The mean value $<\mathcal{H}_0>_0$ can be evaluated by using the equipartition theorem resulting in

$$\langle\mathcal{H}_0\rangle_0 = \frac{Nk_BT}{2}+\frac{Nk_BT}{2} = Nk_BT. \quad (19)$$

On the other hand, the mean value of $<\mathcal{H}>_0$ is not so straightforward computed. It can be written as

$$\langle\mathcal{H}\rangle_0 = -\frac{J}{2}\sum_{\vec{r},\vec{a}}\langle\sqrt{1-(S_{\vec{r}}^z)^2}\sqrt{1-(S_{\vec{r}+\vec{a}}^z)^2}\rangle_0\langle\cos(\phi_{\vec{r}+\vec{a}}-\phi_{\vec{r}})\rangle_0 - \frac{J_z}{2}\sum_{\vec{r},\vec{c}}\langle\sqrt{1-(S_{\vec{r}}^z)^2}\sqrt{1-(S_{\vec{r}+\vec{c}}^z)^2}\rangle_0\langle\cos(\phi_{\vec{r}+\vec{c}}-\phi_{\vec{r}})\rangle_0 + D\sum_{\vec{r}}\langle(S_{\vec{r}}^z)^2\rangle_0, \quad (20)$$

where in the first two sums the mean value of the product of the planar and axial terms regarding the trial Hamiltonian has been factorized and

$$\langle(S_{\vec{r}}^z)^2\rangle_0 = \frac{k_BT}{2(D+2J+J_z)} \quad (21)$$

is the out-of-plane spin fluctuation.

For the Gaussian variables $(\phi_{\vec{r}+\vec{a}}-\phi_{\vec{r}})$ we can write

$$\langle\cos(\phi_{\vec{r}+\vec{a}}-\phi_{\vec{r}})\rangle_0 = e^{-\frac{1}{2}\langle(\phi_{\vec{r}+\vec{a}}-\phi_{\vec{r}})^2\rangle_0}, \quad (22)$$

where the mean value appearing in the exponential is given by

$$\langle(\phi_{\vec{r}+\vec{a}}-\phi_{\vec{r}})^2\rangle_0 = \frac{2}{N}\sum_{\vec{q}}(1-\lambda_{\vec{q}})\langle|\phi_{\vec{q}}|^2\rangle_0, \quad (23)$$

where $\lambda_q = \frac{1}{2}(\cos q_x a+\cos q_y a)$ and

$$\langle|\phi_q|^2\rangle_0 = \frac{k_BT}{2(\gamma_q+\gamma_{qz})}. \quad (24)$$

Similarly, for the Gaussian variable $(\phi_{\vec{r}+\vec{c}}-\phi_{\vec{r}})$ we have

$$\langle\cos(\phi_{\vec{r}+\vec{c}}-\phi_{\vec{r}})\rangle_0 = e^{-\frac{1}{2}\langle(\phi_{\vec{r}+\vec{c}}-\phi_{\vec{r}})^2\rangle_0},$$

and

$$\langle(\phi_{\vec{r}+\vec{c}}-\phi_{\vec{r}})^2\rangle_0 = \frac{2}{N}\sum_{\vec{q}}(1-\lambda_{\vec{q}}^z)\langle|\phi_{\vec{q}}|^2\rangle_0, \quad (25)$$

where $\lambda_{qz} = \cos q_z c$. In this way, Eq. (20) assumes the form

$$\langle\mathcal{H}\rangle_0 = -\frac{J}{2}\sum_{\vec{r},\vec{a}}(1-\langle(S_{\vec{r}}^z)^2\rangle_0)e^{-\frac{1}{N}\sum_{\vec{q}}(1-\lambda_q)\langle|\phi_q|^2\rangle_0} - \frac{J_z}{2}\sum_{\vec{r},\vec{c}}(1-\langle(S_{\vec{r}}^z)^2\rangle_0)e^{-\frac{1}{N}\sum_{\vec{q}}(1-\lambda_{qz})\langle|\phi_q|^2\rangle_0} + \sum_{\vec{q}}D\langle|S_{\vec{q}}^z|^2\rangle_0, \quad (26)$$

where we have used an additional assumption that $S^z_{\vec{r}} \approx S^z_{\vec{r}+\vec{a}}$ and $S^z_{\vec{r}} \approx S^z_{\vec{r}+\vec{c}}$. The last term can again be computed from the equipartition theorem and as the terms in the sums do not depend on the respective indexes we have

$$\langle\mathcal{H}\rangle_0 = -2JN(1-\langle(S^z_{\vec{r}})^2\rangle_0)e^{-\frac{1}{2N}\sum_{\vec{q}}(2-(\cos q_x a+\cos q_y a))\langle|\phi_q|^2\rangle_0} -J_zN(1-\langle(S^z_{\vec{r}})^2\rangle_0)e^{-\frac{1}{N}\sum_{\vec{q}}(1-\cos q_z c)\langle|\phi_q|^2\rangle_0}+\frac{NDk_BT}{2\Omega} \quad (27)$$

The right hand side of Eq. (4) is then written as

$$\Phi(\gamma,\gamma_z) = -\frac{k_BT}{2}\sum_{\vec{q}}\ln\frac{\pi}{\beta(\gamma_q+\gamma_{qz})} - \frac{k_BT}{2}\sum_{\vec{q}}\ln\frac{\pi}{\beta\Omega} -2JN(1-\langle(S^z_{\vec{r}})^2\rangle_0)e^{-\frac{1}{2N}\sum_{\vec{q}}(2-(\cos q_x a+\cos q_y a))\langle|\phi_q|^2\rangle_0} -J_zN(1-\langle(S^z_{\vec{r}})^2\rangle_0)e^{-\frac{1}{N}\sum_{\vec{q}}(1-\cos q_z c)\langle|\phi_q|^2\rangle_0} -(2-\frac{D}{\Omega})\frac{NK_BT}{2} \quad (28)$$

Minimizing the above equation with respect to the variational parameters gives an upper bound limit for the free energy. The variational parameters are determined from the conditions

$$\frac{\partial\Phi(\gamma,\gamma_z)}{\partial\gamma} = 0\ (a) \qquad \text{and} \qquad \frac{\partial\Phi(\gamma,\gamma_z)}{\partial\gamma_z} = 0.\ (b) \quad (29)$$

The mathematical expressions for Eqs. (29) are rather lengthy to be reproduced here. However, factorizing terms that can be canceled out and defining

$$\eta_{xy} = \frac{1}{2N}\sum_{\vec{q}}\left[2-(\cos q_x a+\cos q_y a)\right]\langle|\phi_q|^2\rangle_0, \quad (30)$$

$$\eta_z = \frac{1}{N}\sum_{\vec{q}}(1-\cos q_z c)\langle|\phi_q|^2\rangle_0, \quad (31)$$

we arrive at the following expression

$$\left[1-\langle(S^z_{\vec{r}})^2\rangle_0\right]\left(2J\eta_{xy}e^{-\eta_{xy}}+J_z\eta_z e^{-\eta_z}\right) = \frac{k_BT}{2}. \quad (32)$$

It is interesting to notice that this very same equation is obtained either from condition (29a) or (29b), meaning that both variational parameters cannot be obtained from this equation alone. However, from the Gaussian variable definitions (22)-(25) one can deduce the following additional relation for the fluctuations η_{xy} and η_z

$$2\gamma\eta_{xy}+\gamma_z\eta_z = \frac{k_BT}{2}. \quad (33)$$

Comparing now Eqs. (32) and (33) we end at the following identifications

$$\gamma = J\left[1-\langle(S^z_{\vec{r}})^2\rangle_0\right]e^{-\eta_{xy}}, \quad (34)$$

$$\gamma_z = J_z\left[1-\langle(S^z_{\vec{r}})^2\rangle_0\right]e^{-\eta_z}, \quad (35)$$

which are now two parametric equations from which the two variational parameters can be obtained. These equations can be put in a more convenient form by noting that

$$e^{-\eta_{xy}} = \exp\left\{-\frac{1}{N}\sum_{\vec{q}}\frac{k_BT(1-\lambda_q)}{2\left[2\gamma(1-\lambda_q)+\gamma_z(1-\lambda_{qz})\right]}\right\} \quad (36)$$

Taking the continuum limit of the above equation in cylindrical coordinates $\frac{1}{N}\sum_{\vec{q}} \rightarrow \frac{a^2c}{2\pi^4}\int_0^{2\pi}d\theta\int_0^{\frac{\pi}{a}}qdq\int_{-\frac{\pi}{c}}^{\frac{\pi}{c}}dq_z$ and the long wave length limit $\vec{q}\approx 0$ we find

$$e^{-\eta_{xy}} = \exp\left\{-\frac{k_BT}{2\gamma}\left[\frac{\arctan g^{\frac{1}{2}}}{3g^{\frac{1}{2}}}+\frac{1}{6}-\frac{g}{6}\ln(1+\frac{1}{g})\right]\right\}, \quad (37)$$

where $g = \frac{\gamma_z}{\gamma}$. Analogously we find

$$e^{-\eta_z} = \exp\{-\frac{k_BT}{2\gamma} \times\left[\frac{1}{g}-\frac{1}{3g^{\frac{3}{2}}}\left(2\arctan g^{\frac{1}{2}}+g^{\frac{1}{2}}-g^{\frac{3}{2}}\ln(1+\frac{1}{g})\right)\right]\}, \quad (38)$$

so that the variational parameters are finally obtained from

$$\gamma = J(1-\langle(S^z_{\vec{r}})^2\rangle_o)\exp\{-\frac{k_BT}{2\gamma}[\frac{\arctan g^{\frac{1}{2}}}{3g^{\frac{1}{2}}} + \frac{1}{6}-\frac{g}{6}\ln(1+\frac{1}{g})]\}, \quad (39)$$

$$\gamma_z = J_z(1-\langle(S^z_{\vec{r}})^2\rangle_o)\exp\{-\frac{k_BT}{2\gamma}[\frac{1}{g} - - \frac{1}{3g^{\frac{3}{2}}}(2\arctan g^{\frac{1}{2}}+g^{\frac{1}{2}}-g^{\frac{3}{2}}\ln(1+\frac{1}{g}))]\}. \quad (40)$$

The two equations above can also be obtained by employing the usual SCHA. Thus, for a given value of $t = k_BT/J$, D/J and J_z/J one can solve the non-linear system (39) and (40) to get γ/J and γ_z/J, and from them the desired thermodynamics of the model. For example, by taking the continuum limit in the long wave length regime the x component of the magnetization is given by

$$m = (1-\frac{1}{2}\langle(S^z_{\vec{r}})^2\rangle_0)\exp\{-\frac{k_BT}{2\pi^2\gamma}[\frac{\arctan(g^{\frac{1}{2}})}{g^{\frac{1}{2}}} + \frac{1}{2}\ln(1+\frac{1}{g})]\}. \quad (41)$$

The transition temperature is obtained when the only solution of Eqs. (39) and (40) is $\gamma = \gamma_z = 0$.

TABLE I: *Reduced transition temperatures t_c for the anisotropic XY model in some isotropic limiting cases according to Monte Carlo (MC), series, present approach, and Assumption 1 and Assumption 2 (Ass. 1-2).*

	MC or series	present	Ass. 1-2
$D \to \infty$, $J_z = 0$	0.90[32]	1.472	1.472
$D \to \infty$, $J_z = J$	2.17[33]	2.190	2.207
$D = 0$, $J_z = 0$	0.78(2)[34]	1.076	1.076
$D = 0$, $J_z = J$	1.54(1)[16], 1.55[35]	1.605	1.613

Before exploring possible simpler solutions of Eqs. (39) and (40) and presenting the numerical results, it is worthwhile now to discuss and compare some limiting cases.

Let us consider first $D = 0$. In this case we have the anisotropic XY model. The out-of-plane spin fluctuation takes the form

$$\langle (S_{\vec{r}}^z)^2 \rangle_0 = \frac{k_B T}{4J + 2J_z}, \tag{42}$$

which is the same as that obtained by Costa et al. [16]. The transition temperature for the two-dimensional model $J_z = 0$, as well as the isotropic three-dimensional model $J_z = J$, are also identical to those from reference [16], respectively, $t_c = 1.076$ and $t_c = 1.605$. However, it is worth to stress here that the present approach not only is a generalization over the model treated by Costa et al. [16] to other values of the axial interaction J_z, but also includes, as it will be seen below, the important contribution of the crystal field interaction D.

In the limit $D \to \infty$, as it will be discussed below, we have the planar rotator model. Again, we find the same transition temperature for the two-dimensional model $t_c = 1.472$ and, for the three-dimensional model, $t_c = 2.190$ [16]. The transition temperatures for $D = 0$ and $D \to \infty$ are given in Table I for the isotropic two- and three-dimensional models together with those coming from other approaches.

In addition, the present approximation can also be used to evaluate the behavior of the x component of the magnetization for small axial interaction $J_z \ll J$ and any value of D. In this limit, we also have $g \to 0$ so Eq. (41) gives

$$m \approx \left[1 - \frac{1}{2}\langle (S_{\vec{r}}^z)^2 \rangle_0\right] \left(\frac{\gamma_z}{\gamma}\right)^{\frac{k_B T}{4\pi^2 K}}. \tag{43}$$

For the planar rotator model we have $\langle (S_{\vec{r}}^z)^2 \rangle_0 = 0$ and the above equation should be compared to

$$m \approx \left(\frac{\gamma_z}{\gamma}\right)^{\frac{k_B T}{8\pi K}}, \tag{44}$$

obtained from a SCHA where γ_z/γ plays the role of K_z/K of Ref. [15] and

$$m = \left(\frac{\gamma_z}{\gamma}\right)^{\frac{k_B T}{8\pi J}}, \tag{45}$$

obtained from spin wave theory where now γ_z/γ plays the role of J_z/J of Ref. [36]. The exponent here is not the same, although numerically comparable to other approaches.

3. Numerical Results, Parametric Procedure and Simple Assumptions

Numerical Results

In Figure 1 we have the reduced transition temperature as a function of the anisotropy $\eta = J_z/J$ for $D = 0$. From hereon the present approach means the results obtained by solving the non-linear system of equations (39) and (40) numerically (by using standard iterative procedures) for the variational parameters. As can be seen from this figure the results are quite similar to those from reference [16] in the region close to the isotropic three-dimensional case $J_z \sim J$. On the other hand, the slope of the phase boundary close to isotropic two-dimensional case $J_z = 0$ is zero according to the present approach while the procedure from reference [16] for the XY model (and also for the planar rotator model [15]) furnishes a positive slope.

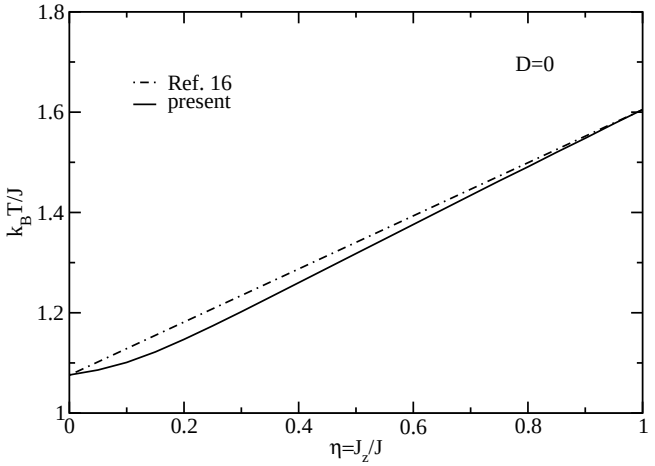

FIG. 1: Reduced transition temperature $t = k_B T/J$ as a function of $\eta = J_z/J$ for $D = 0$. The solid line represents the present approach and the dot-dashed line the results from Ref. [16].

Figure 2 shows the phase diagram in the reduced temperature $t = k_B T/J$ and $\eta = J_z/J$ plane for several values of D/J. One can clearly note that the crystalline anisotropy D plays an important role in the critical behavior of the model.

For positive values of the crystal field $D > 0$ the transition temperature increases as D increases, since in this case the out-of-plane fluctuations are reduced implying a greater tendency of the spin components to lie in the xy plane. For $D \to \infty$ we recover the planar rotator model because there will be no z component of any spin. As shown in Table I, in this limit, the result $t_c = 1.472$ for $J_z = 0$ are quite different from that obtained by Monte Carlo simulations $t_c = 0.90$, reflecting the fact that the present variational approach does not take into account vortices effects, which are relevant for such two-dimensional model. On the other hand, for $J_z = J$ the result $t_c = 2.190$ for the isotropic three-dimensional planar rotator model are quite comparable to the Monte Carlo simulations $t_c = 2.17$. Moreover, in the two-dimensional limit ($J_z = 0$), Eqs. (39) and (40) can be written as

$$\frac{k_B T_c}{J} = t_c = \frac{8 + 4\frac{D}{J}}{2 + e(2 + \frac{D}{J})}, \tag{46}$$

which gives the transition temperature of Fig. 2 for $\eta = 0$ down to the value $\frac{D}{J} = -2$.

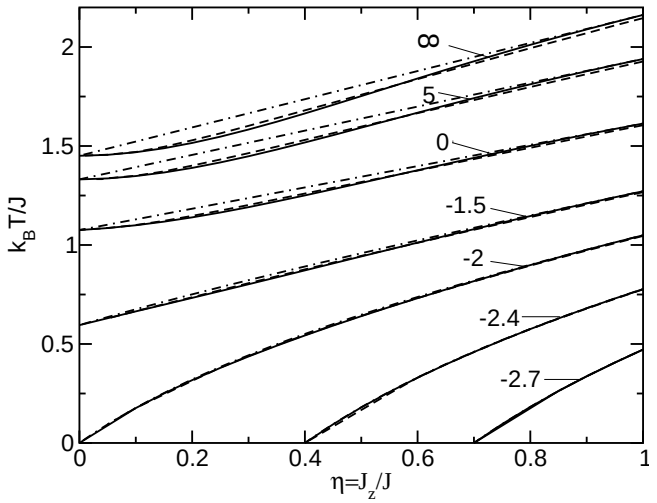

FIG. 2: Reduced transition temperature $t = k_B T/J$ as a function of $\eta = J_z/J$ for several values of D/J (indicated by the numbers) according to the present approach (full lines), and Assumption 1 (dashed lines) and Assumption 2 (dot-dashed lines).

For negative values of the crystal field $D < 0$ we have an inverse situation. We note that as D decreases the transition temperature also decreases. This can be understood because the out-of-plane fluctuations are now enhanced implying in a tendency for the spins to lie out of the xy plane and to become more Ising like. For a given value of D there is a critical value of the ratio $\eta_c = J_z/J$ at which the temperature goes to zero. This value is given by

$$\eta_c = -D/J - 2 \tag{47}$$

at which the out-of-plane fluctuation (21) diverges.

Figures 3 and 4 show the temperature dependence of the magnetization obtained from Eq. (41) where one can see a discontinuous behavior. This discontinuity in the magnetization is an artifact of the present method. The transition temperature is given when the non-linear system of equations (39) and (40) admit only the trivial solution. In all cases they do not go smoothly to the trivial solution presenting thus a discontinuity. This is a general feature of such methods. For instance, the temperature behavior for $D \to \infty$ and $J_z/J = 0.1$ and $J_z/J = 1$ shown in Figure 4 is quite similar to those given in Figure 3 of reference [15].

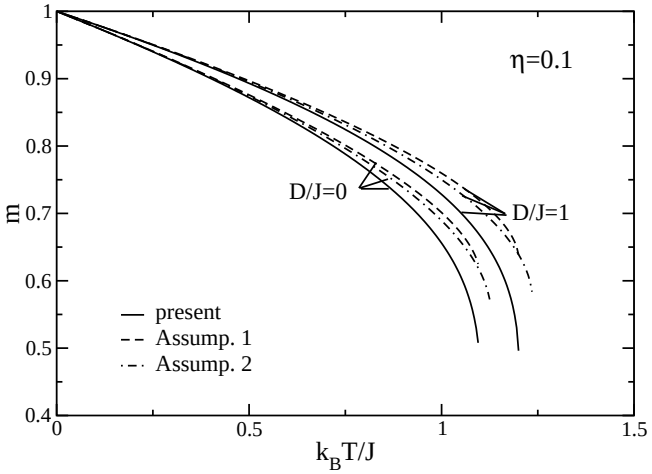

FIG. 3: Magnetization m as a function of the reduced temperature $k_B T/J$ for $\eta = J_z/J = 0.1$ and two different values of the crystal field, $D/J = 0$ and $D/J = 1$, according to the present approach (full lines), and Assumption 1 (dashed lines) and Assumption 2 (dot-dashed lines).

Parametric Procedure and Simple Assumptions

If we take the ratio between the variational stiffness $g = \frac{\gamma_z}{\gamma}$, we can compute the quadratic fluctuations given by Eqs. (30) and (31) by taking the continuum limit in the long wavelength regime

$$\eta_{xy} = \frac{k_B T}{2\gamma} F(g), \qquad \eta_z = \frac{k_B T}{2\gamma} \left[\frac{1 - 2F(g)}{g}\right], \tag{48}$$

where

$$F(g) = \frac{1}{3}\left[\frac{\arctan\left(g^{\frac{1}{2}}\right)}{g^{\frac{1}{2}}} + \frac{1}{2} - \frac{1}{2} g \ln\left(1 + \frac{1}{g}\right)\right]. \tag{49}$$

On the other hand, Eq. (32) can be written as

$$G(Q) = Q \ln Q \left[2 + \eta\alpha Q^{\alpha-1}\right] = \frac{-t}{2\left[1 - \langle (S^z_{\vec{r}})^2 \rangle_0\right]}, \tag{50}$$

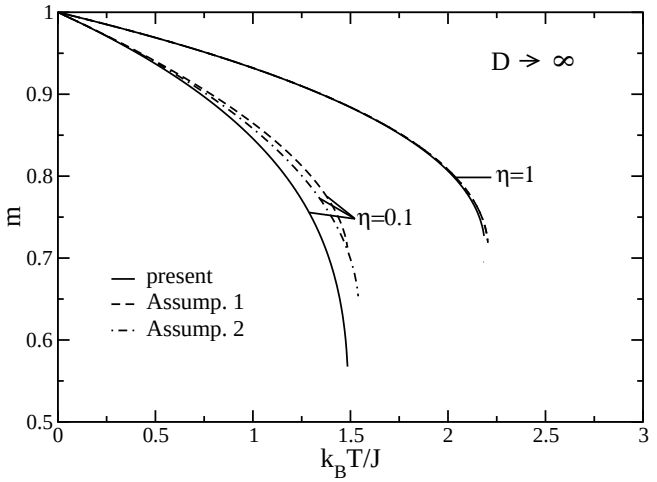

FIG. 4: Magnetization m as a function of the reduced temperature k_BT/J for $D \to \infty$ and two different values of $\eta = J_z/J$, $\eta = 0.1$ and $\eta = 1$, according to the present approach (full lines), and Assumption 1 (dashed lines) and Assumption 2 (dot-dashed lines).

where $Q = e^{-\eta_{xy}}$, $\alpha = \frac{\eta_z}{\eta_{xy}}$ and $\eta = \frac{J_z}{J}$. From Eqs. (48) the parameter α and, in the same way from Eqs. (34) and (35) the quantity Q, can be written in terms of the ratio g as

$$\alpha = \left[\frac{1-2F(g)}{2F(g)}\right], \qquad Q = \left(\frac{g}{\eta}\right)^{\frac{1}{\alpha-1}}. \tag{51}$$

Finally, the temperature can be expressed in terms of $G(Q)$ as

$$t = \frac{-2G(Q)}{1-\frac{J}{\Omega}G(Q)}. \tag{52}$$

So, knowing a priori the Hamiltonian parameters η and D/J and for a given value of g one gets

$$g \to F(g) \to \alpha \to Q \to G(Q) \to t. \tag{53}$$

This is indeed what really happens when we use the numerical solution of the implicit self-consistent equations (39) and (40). However, it would be quite nice if one could track the inverse path of Eq. (53). Unfortunately, as one can see, this is in fact not possible since for a given t (the usual parametric procedure to get the different thermal dependences) we cannot solve Eq. (50) because α is unknown. It is at this point where some additional assumptions could be made in order to explore simpler solutions of Eq. (50).

Assumption 1. $\alpha = \eta$

In this case Eq. (50) reduces to

$$Q \ln Q \left[2+\eta^2 Q^{\eta-1}\right] = \frac{-t}{2\left[1-\langle (S^z_{\vec{r}})^2\rangle_0\right]}. \tag{54}$$

In Figure 2 it is shown, by the dashed lines, the corresponding critical temperatures according to this assumption. It can be seen that, within that scale, Assumption 1 and the present variational approach are almost indistinguishable. For $D = 0$ the transition temperature obtained from Eq. (54) for the two-dimensional model $J_z = 0$ is identical to that from the present one $t_c = 1.076$. However, for the isotropic three-dimensional model $J_z = J$ one has $t_c = 1.613$, which is slightly different from the value $t_c = 1.605$ according to reference [16]. On the other hand, in the limit $D \to \infty$ we find the same transition temperature for the two-dimensional planar rotator model $t_c = 1.472$ and, for the three-dimensional case, $t_c = 2.207$ is comparable to $t_c = 2.190$ obtained from Ref. [16]. These values are depicted in Table I together with those coming from other approaches. The magnetization as a function of the temperature is presented in Figures 3 and 4. A different behavior is observed, except for the planar rotator model.

The quite good agreement of the present approach and Assumption 1 reflects the fact that the term $\eta\alpha Q^{\alpha-1}$ in Eq. (50) varies very weakly with g and thus with temperature. Reproducing the correct limits at $\eta = 0$ and 1 the phase boundaries are then a sort of smooth interpolation for different values of the anisotropy, explaining the accidental good agreement. With this in mind other simplifications can also be done.

Assumption 2. $F(g) = \frac{1}{2+g}$

In the interval $[0, 1]$, the function $F(g)$ given by Eq. (49) can be approximated by (with an error of order less than 10%)

$$F(g) = \frac{1}{2+g}. \tag{55}$$

This implies that $\alpha = 1$ and $\eta_z = \eta_{xy}$, meaning that the quadratic fluctuations are not very different in vertical or in-plane bonds. The self-consistent Eq. (50) adopts now a very simple form

$$Q \ln Q \,[2+\eta] = \frac{-t}{2\left[1-\langle (S^z_{\vec{r}})^2\rangle_0\right]}. \tag{56}$$

Unlike Eq. (54) the above equation permits obtaining an analytical expression for the critical temperature. Since $\frac{dQ}{dt} = 0$ at t_c one gets $Q_c = e^{-1}$ and

$$t_c = \frac{2(2+\eta)}{\frac{J}{\Omega}(2+\eta)+e}. \tag{57}$$

The above equation also yields exactly the same limiting results as in the last column of Table I. The boundaries as a function of D are given in Figure 2 by the dot-dashed lines. In this case, for positive values of the crystal anisotropy the agreement is not as good as for negative values. The corresponding magnetizations as a function of the temperature are also shown in Figures 3 and 4.

4. CONCLUDING REMARKS

The anisotropic XY model in a crystalline field has been studied according to a variational approach for the free energy. This system is a generalization of the planar rotator model and the anisotropic XY model previously treated in the literature [15, 16]. We believe we have obtained a satisfactory picture of the thermodynamic behavior of the model as a function of its parameters. Not only is the phase diagram in the anisotropic case $J_z \neq J$ different from the previous one obtained for $D = 0$, but the crystal field has been show to play an important role in the critical behavior of the system.

Regarding Assumptions 1 and 2, one could see that the former one ($\alpha = \eta$) would imply that the mean quadratic fluctuation on a given bond scales with the coupling constant of the bond, while the latter one ($\alpha = 1,\ \eta = 1$) means that the quadratic fluctuations are not very different in vertical or in-plane bonds. So, according to Assumption 2, the average contribution to the internal energy from each bond scales approximately with the coupling constant of the considered bond. This seems more acceptable than the conceptually wrong assumption $\alpha = \eta$, since one expects that softer bonds should develop stronger fluctuations. Thus, at first sight, from the numerical point of view, the better agreement of Assumption 1 with the complete approach can be ascribed to an artifact of the method.

It is clear from the approximation employed in this work that it should be valid only at low temperatures. It is also rather surprising that the values for the transition temperatures shown in Table I for the three-dimensional model are quite comparable to those coming from more reliable methods (for the two dimensional model one would not expect such agreement due to the vortices effects). It would then be quite nice to have a clearer picture of the range of the temperature validity of the present procedure. In Figure 5 we show the out-of-plane spin fluctuations given by Eq.(21) for several values of the Hamiltonian parameters compared to Monte Carlo simulations. We have chosen this quantity because it is easily obtained from the present approximation, Eq.(21). The simulations have been done in the three-dimensional model described by Hamiltonian (1) and employing the single spin-flip Metropolis algorithm. A finite lattice of $L \times L \times L$ ($L = 14$) has been used with periodic boundary conditions. The averages have been taken by considering 10^5 Monte Carlo steps (MCS) per spin after equilibration. For the first temperature, $100L^2$ MCS have been discarded and, with the previous configuration being the initial configuration for the next temperature, additional 3×10^3 have been discarded. It is evident from this figure that the transition temperatures are not far from the temperature range where the corresponding results are comparable to the Monte Carlo simulations.

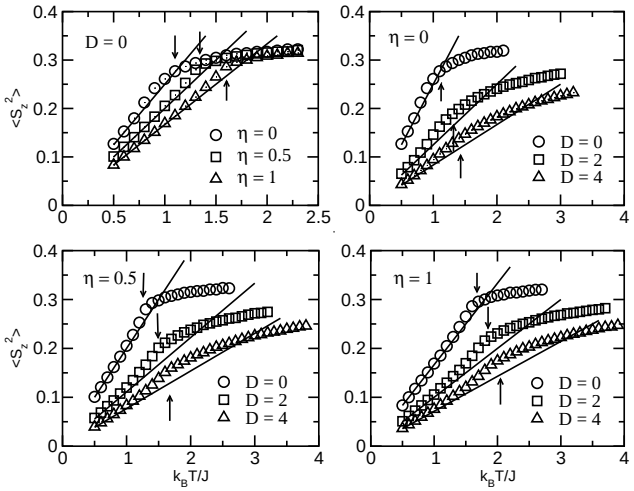

FIG. 5: Out-of-plane spin fluctuation as a function of the temperature for several values of the Hamiltonian parameters. The full lines are the results from Eq. (21) and the different symbols are Monte Carlo simulations [37]. The arrows indicate the transition temperatures obtained from the present approximation. The MC results saturates at 1/3 as $T \to \infty$.

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